

Abstract Submitted
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Atomistic modeling of the sodium diffusion in black phosphorus anode. SAEID ARABNEJAD KHANOOKI, researcher, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, SHUNSUKE KURAHASHI, Master Student, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, KOICHI YAMASHITA, Professor, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, YAMASHITA USHIYAMA LAB. TEAM — The increasing demand for rechargeable batteries and limitations in lithium resources has encouraged material scientists to search for alternative materials and systems for the next generation of batteries. Phosphorus-sodium systems with high theoretical capacity of 2596 mAhg^{-1} seems to be one of the best feasible choices. Although the structure and properties of pure Phosphorus and fully Sodiated phosphorus (Na_3P) are well known, the characteristics of intermediate phases are not well established. In this study we try to identify these phases and characterize their properties using two sub-atomic computational schemes. Density functional theory (DFT) and density functional tight binding (DFTB) are employed in this study. DFT has been incorporated to measure the chemical shift of different suggested phases and results have been compared with the available NMR results. It also has been observed that some of these phases are not stable when subjected to relatively small mechanical deformation. For a more realistic simulation of diffusion process, larger atomic models are preferred and therefore, DFTB has been employed for this part of the study. The DFTB parameters are initially modified based on the DFT results and then applied for the diffusion simulation.

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